# Mesoscale Simulations of Crack Propagation

*V. Dwivedi [University of California at Santa Barbara (UCSB)/T-11]; Rajeev Ahluwalia, Turab Lookman, and Avadh Saxena (T-11); and S. Bannerjee (UCSB)*

Fracture patterns show signs of coherent dynamical behavior. For example, after a short transient, the speed of a propagating crack often reaches some limiting average speed. When the crack speed is still low, the crack surface is usually rather smooth. However, when the speed is above a threshold value of the order of the asymptotic speed, the crack surface suddenly becomes much rougher and the crack speed often exhibits strong fluctuations. Above the critical speed, inspection of the crack surface shows that the crack branches. Fast crack growth in brittle solids typically reveals complex patterns of crack branching; for example, the shattering from a rock impact of a plastic that leads to a pattern of repeated branching of a crack into multiple side-branches. Supporting numerical analysis at the continuum level, using finite-element methods based on prescribed cohesive laws to govern the separation of surfaces under the tensile mode, reveals the effect of the crack propagation speed on the branching and surface roughness characteristics of such fast moving cracks.

What makes a theoretical or numerical analysis of crack propagation difficult is that one cannot use continuum elastic theory alone. A continuum elastic theory in which the crack is taken as a mathematically sharp cut is prone to singular behavior—one really has to put in the breaking of bonds or the dissipation of energy near the crack tip into the model to obtain a proper description. Numerically it has indeed become possible, in recent years, to do large-scale molecular dynamics simulations (sometimes matched to continuum elastic models on large scales), which do reproduce many of the experimental features, including the splitting of cracks. However, from such simulations it is still difficult to separate the essentially long-range dynamical behavior from what is intrinsic to a particular short-range molecular potential.

Recently, we have studied mesoscale models based on local Landau potentials to describe crack dynamics. The model introduces a continuum order parameter or "phase field" to describe a stiff solid or a broken material which does not support stresses, and which interpolates between these two extremes in a thin zone. In the present context, this transition zone is the "process zone" where the breaking occurs. Within such a model, the atomistic breaking of bonds is not incorporated realistically, but it is mimicked by having energy dissipate there. The numerical advantage of such models is that their simulations are relatively simple, and they allow one to study coherent behavior, which is independent of the precise atomistic details. Also, they allow for computations to realistic length and time scales.

The problem we consider is a very thin plate with an initial central crack under a Mode I fracture. Plain strain conditions are assumed to exist. A tensile loading is applied through an imposed strain field. The material is assumed to be elastic; we consider both the isotropic case as would apply to a brittle plastic such as PMMA (poly-methyl-methacrylate) and anisotropic case for a system with two-dimensional square symmetry that is uniform in the third direction. Our model contains dynamics derived using force balance with inertial and dissipative effects included. Phase field models have not previously been applied to study branching or crack propagation. Our objective is to show the efficacy of the method in modeling not only the natural initiation and growth of the crack, but also the branching characteristics and the effect of branching on the mechanical strength of the material.

Figure 1 shows how a crack evolves as a function of a time varying strain, using an applied strain rate of 0.005 in the normal direction. The initial crack shape is elliptical with length less than a tenth of the width seeded at the center. The dark regions

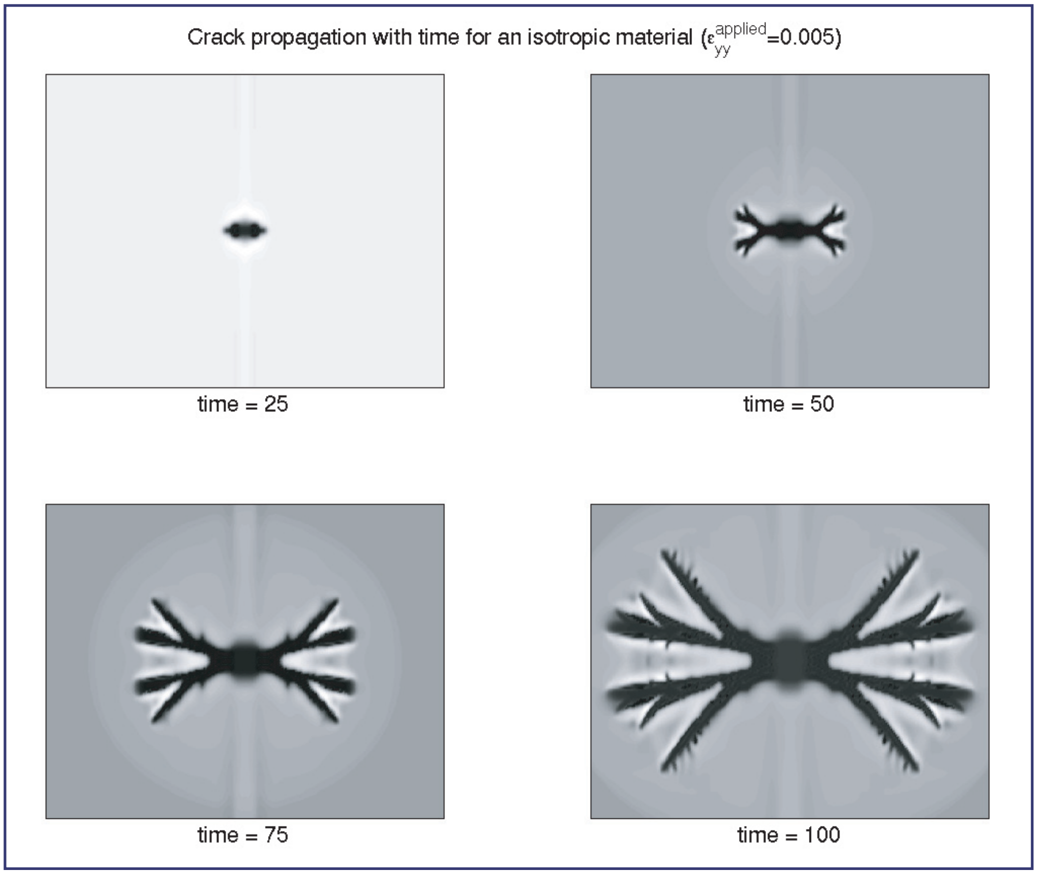


*Figure 1—*
***The figure shows how a crack evolves as a function of a time varying strain, using an applied strain rate of 0.005 in the normal direction. The dark regions represent the crack.***

represent the crack. Stresses develop near the crack tips, which start to grow once the imposed strain reaches a critical value. The crack rapidly side-branches and even these subbranches break up readily.

***For more information, contact Turab Lookman (txl@lanl.gov).***

**Acknowledgements**
We would like to acknowledge NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program for financial support.